

Spectrum of Three-Body Bound States in a Finite Volume

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(Received 12 January 2015; revised manuscript received 4 February 2015; published 4 March 2015)

The spectrum of a bound state of three identical particles with a mass m in a finite cubic box is studied. It is shown that in the unitary limit, the energy shift of a shallow bound state is given by $\Delta E = c(\kappa^2/m)(\kappa L)^{-3/2}|A|^2 \exp(-2\kappa L/\sqrt{3})$, where κ is the bound-state momentum, L is the box size, $|A|^2$ denotes the three-body analog of the asymptotic normalization coefficient of the bound state wave function, and c is a numerical constant. The formula is valid for $\kappa L \gg 1$.

DOI: 10.1103/PhysRevLett.114.091602

PACS numbers: 11.10.St, 11.80.Jy, 12.38.Gc

Introduction.—Strong interactions between two particles can be studied in *ab initio* lattice simulations, like for hadron-hadron scattering in quantum chromodynamics or dimer-dimer scattering at ultracold temperatures. At present, Lüscher's approach [1] represents a standard way to study two-body scattering observables on the lattice. In its original form, this approach relates the two-particle scattering phase in the elastic region to the measured energy spectrum of the Hamiltonian in a finite volume. In the literature, one finds different generalizations of the Lüscher approach. For instance, the approach has been formulated in the case of moving frames [2], (partially) twisted boundary conditions [3], and for coupled-channel scattering [4] (for a recent application of this approach to the analysis of the two-channel case on the lattice, see Ref. [5]). A closely related framework based on the use of the unitarized ChPT in a finite volume has also been proposed [6]. Further, a method for the measurement of resonance matrix elements and form factors in the timelike region has been worked out [7]. Note, however, that all of these generalizations explicitly deal with two-body channels. Studying a genuinely three-body problem in a finite volume has proven to be a far more complicated enterprise and, albeit there have been several attempts to solve this problem in the past few years [8–13], the method is still in its infancy. On the other hand, recent progress on the lattice, related to the study of the inelastic resonances such as the Roper resonance [14] and of the properties of light nuclei [15–17], indicates that the generalization of the Lüscher method to the multiparticle (three and more) systems is urgently needed.

The main obstacle that one encounters in generalizing Lüscher's approach from two to three particles has a transparent physical interpretation. In the center-of-mass (c.m.) frame, the two-body scattering can be considered as a scattering of one particle in a given potential. If this potential has a short range (much smaller than the box size L), then

the scattering wave function at the boundaries will depend only on the scattering phase shift in the infinite volume and, therefore, the discrete spectrum in a finite box will be determined by this phase shift only. In other words, the spectrum in a large but finite box does not depend on the details of the interaction at short distances. This is not so obvious in the case of three particles. In this case, each pair of particles can come close to each other and still be separated from the third one by a large distance of order L . It took a certain effort to prove that, despite the fact that such configurations are allowed, the finite-volume spectrum is still determined solely by the infinite-volume S -matrix elements and does not depend on the short-range details of the interaction [8]; see also Refs. [9,10]. For instance, in a recent paper [9], the authors succeeded in deriving a quantization condition for the three-particle spectrum in a finite volume. It has a quite complicated structure, in particular, due to the fact that the infinite-volume amplitudes that enter this condition are defined in an unconventional manner (the necessity of such a definition has been pointed out already in Ref. [8]). For this reason, it is not an easy task to use this quantization condition for the analysis of lattice data—in fact, we are not aware of a single explicit prediction for the volume dependence of physical observables except for the ground-state shift of identical particles [18], which was done in this formalism [19]. Note also that in Ref. [13], in the framework of the nonrelativistic effective field theory, it has been explicitly demonstrated that carrying out the renormalization in the infinite volume leads to the cutoff-independent three-particle bound-state spectrum in a finite volume that is equivalent to the statement that this spectrum is determined by the S -matrix elements in the infinite volume.

The aim of this Letter is to obtain such an explicit volume dependence for the physical quantity that, in our opinion, is the easiest to handle. In particular, we consider shallow bound states of three identical particles in the

unitary limit. This means that the two-body scattering length a tends to infinity and the corresponding effective range is zero. The three-body bound-state momentum κ , which is related to the binding energy E_T through $E_T = \kappa^2/m$, is much smaller than the particle mass m or the inverse of the interaction range. Still, we consider large boxes where $\kappa L \gg 1$. Our treatment of the three-body bound state is not based on the quantization condition derived in Ref. [9], but closely follows the two-body pattern of Ref. [20] (see also Refs. [12,21], where, in particular, the result of Ref. [20] is generalized to the case of an arbitrary angular momentum). For this reason, our explicit result provides a beautiful testing ground for the general approach formulated in Ref. [9] and helps us to better understand its structure. On the other hand, our result can be immediately verified through numerical calculations in a finite volume similarly to those carried out, e.g., in Ref. [13] that provides an additional check on the theoretical framework.

Derivation of the formula for energy shift.—We start from the Schrödinger equation for three identical particles in the infinite volume,

$$\left\{ \sum_{i=1}^3 \left(-\frac{1}{2m} \nabla_i^2 + V(\mathbf{x}_i) \right) + E_T \right\} \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = 0, \quad (1)$$

where $\nabla_i = \partial/\partial \mathbf{r}_i$ and the Jacobi coordinates are defined as

$$\mathbf{x}_i = \mathbf{r}_j - \mathbf{r}_k, \quad \mathbf{y}_i = \frac{1}{\sqrt{3}}(\mathbf{r}_j + \mathbf{r}_k - 2\mathbf{r}_i), \quad (2)$$

with $(ijk) = (123), (312), (231)$. Here, for simplicity, we assume that no three-body force is present. The inclusion of the latter can be done in analogy with Ref. [8].

In a finite volume, the potential V is replaced by a sum over all mirror images

$$V_L(\mathbf{x}_i) = \sum_{\mathbf{n} \in \mathbb{Z}^3} V(\mathbf{x}_i + \mathbf{n}L), \quad (3)$$

and the Schrödinger equation takes the form

$$\left\{ \sum_{i=1}^3 \left(-\frac{1}{2m} \nabla_i^2 + V_L(\mathbf{x}_i) \right) + E_L \right\} \psi_L(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = 0. \quad (4)$$

In the c.m. frame, the bound-state wave functions ψ, ψ_L depend on two Jacobi coordinates $\mathbf{x}_i, \mathbf{y}_i$. For three identical particles, $\psi(\mathbf{x}_i, \mathbf{y}_i) = \psi(\mathbf{x}_k, \mathbf{y}_k)$, $i, k = 1, 2, 3$, and similarly to the finite-volume wave function ψ_L .

In order to evaluate the finite-volume shift $\Delta E = E_T - E_L$, in analogy to Ref. [20], we define in the c.m. frame the trial wave function (we choose $i = 1$ from now on)

$$\psi_0 = \sum_{\mathbf{n}, \mathbf{m}} \psi \left(\mathbf{x}_1 - (\mathbf{n} + \mathbf{m})L, \mathbf{y}_1 + \frac{1}{\sqrt{3}}(\mathbf{n} - \mathbf{m})L \right). \quad (5)$$

Denoting $H_L = \sum_{i=1}^3 [-(1/2m)\nabla_i^2 + V_L(\mathbf{x}_i)]$, it can be straightforwardly checked that ψ_0 obeys the equation $(H_L + E_T)\psi_0 = \eta$, where

$$\eta = \sum_{\mathbf{n}, \mathbf{m}} \hat{V}_{\mathbf{n}\mathbf{m}} \psi \left(\mathbf{x}_1 - (\mathbf{n} + \mathbf{m})L, \mathbf{y}_1 + \frac{1}{\sqrt{3}}(\mathbf{n} - \mathbf{m})L \right) \quad (6)$$

and

$$\begin{aligned} \hat{V}_{\mathbf{n}\mathbf{m}} = & \sum_{\mathbf{k} \neq -\mathbf{n}-\mathbf{m}} V(\mathbf{x}_1 + \mathbf{k}L) + \sum_{\mathbf{k} \neq \mathbf{n}} V(\mathbf{x}_2 + \mathbf{k}L) \\ & + \sum_{\mathbf{k} \neq \mathbf{m}} V(\mathbf{x}_3 + \mathbf{k}L). \end{aligned} \quad (7)$$

Since the potential $V(\mathbf{x})$ has a short range, the quantity η exponentially vanishes at a large L , $\eta \propto \exp(-\text{const} \times \kappa L)$. Further, applying perturbation theory, it can be verified that, to all orders, the energy shift is given by

$$\begin{aligned} \Delta E = & \frac{\langle \psi_0 | T | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}, \\ T = & (H_L + E_T) - (H_L + E_T) Q G Q (H_L + E_T), \end{aligned} \quad (8)$$

where

$$G = \frac{1}{H_L + E_L}, \quad Q = \frac{|\psi_0\rangle\langle\psi_0|}{\langle\psi_0|\psi_0\rangle}. \quad (9)$$

Since the quantity η is exponentially suppressed at a large L , the leading exponential correction to the energy shift is given by (cf. Ref. [20])

$$\Delta E = \frac{\langle \eta | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} + \dots \quad (10)$$

Note that in Ref. [12] this formula in the case of more than two particles was given without derivation. A detailed derivation in the case of two particles is given in Ref. [21].

In the next step, one substitutes the expression for η from Eq. (6) into the above expression for the energy shift and picks those terms that give a leading exponential contribution at large L . Taking into account the fact that the argument of the exponent in the infinite-volume wave function $\psi(\mathbf{x}_1, \mathbf{y}_1)$ is proportional to the hyperradius $R = (1/\sqrt{2})(\mathbf{x}_1^2 + \mathbf{y}_1^2)^{1/2}$, one has to minimize the sum of two hyperradii, coming from two wave functions in the overlap integral. Finally, the expression of the energy shift at leading order takes the form

$$\begin{aligned} \Delta E = & 6 \times 2 \times 3 \int d^3 \mathbf{x}_1 d^3 \mathbf{y}_1 \psi(\mathbf{x}_1, \mathbf{y}_1) V(\mathbf{x}_1) \\ & \times \psi \left(\mathbf{x}_1 - \mathbf{e}L, \mathbf{y}_1 + \frac{1}{\sqrt{3}}\mathbf{e}L \right) + \dots, \end{aligned} \quad (11)$$

where $\mathbf{e} = (0, 0, 1)$ denotes a unit vector and the ellipses stand for the exponentially suppressed terms. In this

formula, the infinite-volume wave function ψ is normalized to unity. The factor in front of the integral reflects the symmetries: 6 for different orientations of the unit vector \mathbf{e} , 2 for different signs in the second argument of the wave function $\mathbf{y}_1 \pm (1/\sqrt{3})\mathbf{e}L$, and 3 for three different pair potentials.

Evaluation of the energy shift.—In order to evaluate the overlap integral that defines the leading-order energy shift, an explicit expression for the bound-state wave function should be supplied. Only the asymptotic tail of the wave function matters, since the finite-volume spectrum is uniquely determined by the S -matrix elements in the infinite volume [8]. Here, we shall be working in the unitary limit. In the context of the lattice this means that the two-body scattering length $a \geq L$, i.e., even at the box boundaries, the hyperradius $R \leq a$. On the other hand, we assume that the interaction range is much smaller than L . Under these assumptions, almost everywhere in the configuration space, the wave function can be approximated by the well-known universal expression (see, e.g., Ref. [22])

$$\begin{aligned} \psi(\mathbf{x}_1, \mathbf{y}_1) &= A\mathcal{N}R^{-5/2}f_0(R) \sum_{i=1}^3 \frac{\sinh[s_0(\pi/2 - \alpha_i)]}{\sin(2\alpha_i)} \\ &\doteq \sum_{i=1}^3 \phi(R, \alpha_i), \end{aligned} \quad (12)$$

where

$$f_0(R) = R^{1/2}K_{is_0}(\sqrt{2}\kappa R) \quad (13)$$

and $K_\nu(z)$ denotes the Bessel function. Here, $\alpha_i = \arctan(|\mathbf{x}_i|/|\mathbf{y}_i|)$ are Delves hyperangles and the numerical constant $s_0 \approx 1.00624$ is the solution to the transcendental equation

$$s_0 \cosh \frac{\pi s_0}{2} = \frac{8}{\sqrt{3}} \sinh \frac{\pi s_0}{6}. \quad (14)$$

Further, \mathcal{N} is the normalization coefficient of the exact asymptotic wave function in Eq. (12), so that

$$\int d^3\mathbf{x}_1 d^3\mathbf{y}_1 |\psi(\mathbf{x}_1, \mathbf{y}_1)|^2 = |A|^2. \quad (15)$$

Evaluating the integral explicitly, one gets

$$\begin{aligned} \mathcal{N}^2 &= \kappa^2 C_0, \\ C_0^{-1} &= \frac{8\pi^3}{\sinh(\pi s_0)} \left(\frac{3}{4} \sinh(\pi s_0) - \frac{3\pi s_0}{4} \right. \\ &\quad \left. - \frac{4\pi}{\sqrt{3}} \sinh \frac{\pi s_0}{3} + \frac{2\pi}{\sqrt{3}} \sinh \frac{2\pi s_0}{3} \right). \end{aligned} \quad (16)$$

Finally, the quantity $|A|^2$ denotes a three-body analog of the asymptotic normalization coefficient for the wave function. It encodes the information about the short-range dynamics

in the system. Namely, if in the creation of the bound state the long-range effects dominate, it is expected that the quantity $|A|^2$ is close to one [23].

Next, we evaluate the overlap integral in Eq. (11) by using the explicit wave function from Eq. (12). In analogy to Eq. (12), the second wave function in the integral can be written as

$$\psi\left(\mathbf{x}_1 - \mathbf{e}L, \mathbf{y}_1 + \frac{1}{\sqrt{3}}\mathbf{e}L\right) = \sum_{i=1}^3 \phi(R', \alpha'_i). \quad (17)$$

As $L \rightarrow \infty$,

$$R' = \frac{[(\mathbf{x}_1 - \mathbf{e}L)^2 + (\mathbf{y}_1 + \mathbf{e}L/\sqrt{3})^2]^{1/2}}{\sqrt{2}} \rightarrow \sqrt{\frac{2}{3}}L, \quad (18)$$

whereas the angular variables tend to the following limiting values:

$$\begin{aligned} \tan \alpha'_1 &= \frac{|\mathbf{x}_1 - \mathbf{e}L|}{|\mathbf{y}_1 + \mathbf{e}L/\sqrt{3}|} \rightarrow \sqrt{3} + \dots, \\ \tan \alpha'_2 &= \frac{|\mathbf{x}_2 + \mathbf{e}L|}{|\mathbf{y}_2 + \mathbf{e}L/\sqrt{3}|} \rightarrow \sqrt{3} + \dots, \\ \tan \alpha'_3 &= \frac{|\mathbf{x}_3|}{|\mathbf{y}_3 - 2\mathbf{e}L/\sqrt{3}|} \rightarrow \frac{\sqrt{3}}{2} \frac{|\mathbf{x}_3|}{L} + \dots \\ &= \frac{\sqrt{6}R \sin \alpha_3}{2L} + \dots. \end{aligned} \quad (19)$$

The expansion of the angular part of the second wave function yields

$$\sum_{i=1}^3 \frac{\sinh[s_0(\pi/2 - \alpha'_i)]}{\sin(2\alpha'_i)} \rightarrow \frac{L}{\sqrt{6}R} \frac{\sinh(\pi s_0/2)}{\sin(\alpha_3)} + \dots. \quad (20)$$

Using the Faddeev equation

$$\psi(\mathbf{x}_1, \mathbf{y}_1)V(\mathbf{x}_1) = \left[\frac{1}{m} \left(\frac{\partial^2}{\partial \mathbf{x}_i^2} + \frac{\partial^2}{\partial \mathbf{y}_i^2} \right) - E_T \right] \phi(R, \alpha_1), \quad (21)$$

the expression for the overlap integral in the hyperspherical coordinates can be rewritten as

$$\begin{aligned} \Delta E &= 6^{3/2}L \sinh(\pi s_0/2) A\mathcal{N} \left(\sqrt{\frac{2}{3}}L \right)^{-5/2} \\ &\quad \times \sqrt{\frac{\pi}{2}} \exp\left(-\frac{2\kappa L}{\sqrt{3}}\right) \frac{1}{(\sqrt{2}\kappa)^{1/2}} \\ &\quad \times 2 \int R^5 dR \sin^2(2\alpha_1) d\alpha_1 d\Omega_{\mathbf{x}_1} d\Omega_{\mathbf{y}_1} \frac{1}{R \sin \alpha_3} \\ &\quad \times \left[\frac{1}{m} \left(\frac{\partial^2}{\partial \mathbf{x}_i^2} + \frac{\partial^2}{\partial \mathbf{y}_i^2} \right) - E_T \right] \phi(R, \alpha_1). \end{aligned} \quad (22)$$

Here, we have used the asymptotic expression for the hyperradial wave function

$$f_0\left(\sqrt{\frac{2}{3}}L\right) \rightarrow \sqrt{\frac{\pi}{2}} \exp\left(-\frac{2\kappa L}{\sqrt{3}}\right) \frac{1}{(\sqrt{2\kappa})^{1/2}} + \dots \quad (23)$$

Integrating by parts and averaging over solid angles with the use of the following formula,

$$\int d\Omega_{\mathbf{x}_1} d\Omega_{\mathbf{y}_1} \frac{1}{\sin \alpha_3} = \frac{64\pi^2}{\sqrt{3} \sin(2\alpha_1)} \left\{ \sin \alpha_1 \theta \left(\frac{\pi}{3} - \alpha_1 \right) + \sqrt{3} \cos \alpha_1 \theta \left(\alpha_1 - \frac{\pi}{3} \right) \right\}, \quad (24)$$

we arrive at the final result,

$$\Delta E = c(\kappa^2/m)(\kappa L)^{-3/2}|A|^2 \exp(-2\kappa L/\sqrt{3}) + \dots, \quad (25)$$

where

$$c = -144 \times 3^{1/4} \pi^{7/2} C_0 \frac{\sinh^2(\pi s_0/2)}{\cosh(\pi s_0/2)} \simeq -87.886, \quad (26)$$

and the ellipses stand for the subleading terms in L , both exponentially and power-suppressed ones. Note that this behavior qualitatively agrees with the result given in Ref. [13], albeit a more detailed numerical study of the problem is needed.

Equation (25) is the main result of this paper. Measuring the binding energy at different volumes, one may determine the infinite-volume quantities E_T and $|A|^2$ through the extrapolation procedure.

Conclusions.—Equation (25) is an explicit prediction of the volume dependence for a genuine three-body observable. This dependence can be readily verified by using numerical methods that represent a highly nontrivial check of the whole approach. Moreover, understanding the present result in the more general context of the three-body quantization condition, one may gain insight into the complicated three-body formalism. In view of the recent progress in the study of inelastic resonances and nuclei in lattice QCD, this kind of information will be very important.

As mentioned above, the present result is valid within certain approximations. In the future, we plan to go beyond these approximations. For example, the next step could be to study the effects of the partial-wave mixing in the three-particle systems as well as the effects of a finite scattering length and interaction range. Further, it would be extremely interesting (and much more challenging) to address the observables from the scattering sector as well.

The authors would like to thank S. Bour, M. Döring, E. Epelbaum, H.-W. Hammer, M. Hansen, M. Jansen, D. Lee, and S. Sharpe for useful discussions. This work is partially supported by the EU Integrated Infrastructure Initiative

HadronPhysics3 Project under Grant Agreement No. 283286. We also acknowledge support by the DFG (CRC 16, “Subnuclear Structure of Matter” and CRC 110, “Symmetries and the Emergence of Structure in QCD”) and by the Shota Rustaveli National Science Foundation (Project No. DI/13/02). This research is supported in part by Volkswagenstiftung under Contract No. 86260.

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